

1,2,3,5-Tetrachlorobenzene
634-90-2 | DTXSID1026089

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 1.59e-05 mol/L

Global applicability domain: Inside

Local applicability domain index: 6.70e-01

Confidence level: 4.97e-01

Nearest Neighbors from the Training Set

Image not found

Hexachlorocyclopentadiene

Measured: 6.60e-06

Predicted: 9.10e-06

Image not found

Ethane, 1,2-diiodo-

Measured: 6.06e-04

Predicted: 1.27e-03

Image not found

Hexachloropropene

Measured: 6.84e-05

Predicted: 2.12e-04

Image not found

Octachlorocyclopentene

Measured: 2.91e-07

Predicted: 1.00e-06

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Hexachloro-1,3-butadiene

Measured: 1.23e-05

Predicted: 1.79e-05